

Non-adiabatic transport in a quantum dot turnstile

Valeriu Moldoveanu,¹ Vidar Gudmundsson,² and Andrei Manolescu¹

¹*National Institute of Materials Physics, P.O. Box MG-7, Bucharest-Magurele, Romania*

²*Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland*

We present a theoretical study of the electronic transport through a many-level quantum dot driven by time-dependent signals applied at the contacts to the leads. If the barriers oscillate out of phase the system operates like a turnstile pump under a finite constant bias, as observed in the experiments of Kouwenhoven *et al.* [Phys. Rev. Lett. **67**, 1626 (1991)]. The time-dependent currents and their averages over successive pumping periods are computed from the Keldysh formalism for tight-binding models. The calculation considers a sudden application of the pumping potentials at $t = 0$ which leads to transient features of the time-dependent and averaged currents during the first pumping cycles which turn out to be important in the high-frequency regime. We show that in the transient regime the efficiency of the system as a pump is rather poor because it mainly absorbs charge from both leads in order to fill the levels located below the bias window. Under a finite bias and a low-frequency pumping signal the charge transferred across the system depends on the number of levels located within the bias window. The internal charge dynamics and the role of energy sidebands are investigated. The so called satellite peaks of the averaged current are observed also in the transient regime.

PACS numbers: 73.23.Hk, 85.35.Ds, 85.35.Be, 73.21.La

I. INTRODUCTION

The ability to control the transport properties of semiconductor quantum dots by time-dependent perturbations (e.g. microwave signals or optical pulses) allows the observation of photon-assisted tunneling, charge pumping^{1,2,3} and coherent Rabi oscillations.⁴ Also, pump-and-probe techniques were used to estimate relaxation rates and to control spins in quantum dots.⁵ A common point of these experiments is that the time-dependent driving potential is applied *on* the system itself, i.e. on a central metallic gate defining the quantum dot.

Some time ago Kouwenhoven *et al.*⁶ proposed a different setup, in which a quantum dot is coupled to source and drain reservoirs by oscillating tunneling barriers. Technically this is achieved by applying radio-frequency signals to the metallic gates that control the opening of the quantum dot to its surroundings. The two barriers at the contacts are varied in such a way that the system undergoes a cyclic transformation and, under a constant bias applied on the leads, an integer number of electrons is transmitted during one cycle. Therefore the system operates as a turnstile pump. An important feature of the turnstile configuration is that the pumped current has a definite direction due to the finite bias. We remind here that originally the concept of parametric charge pumping was introduced in the context of a net current generation in an *unbiased* system.⁷ As noted in the literature, a symmetry breaking is necessary in order to get a nonvanishing current without a bias. In spite of the fact that the turnstile operation was experimentally observed some time ago, it attracted little attention in the theoretical literature (see Refs. 10,13,14,17 below). The purpose of this work is to explore the transport properties of turnstile quantum dots submitted to time-dependent signals

of arbitrary amplitude and frequency.

At theoretical level the quantum pumping was discussed basically within two frameworks: the adiabatic or Floquet scattering theory^{7,8,9,11} and the non-equilibrium Green-Keldysh formalism.^{14,15,16,17} The scattering approach was primarily designed to describe the adiabatic pumping, in which the driving potential varies very slowly. The timescale on which the applied signal varies significantly exceeds the time needed for the electron to pass through the system. The key result of the adiabatic scattering is a current formula in terms of an instantaneous (frozen) S matrix. This matrix is computed perturbatively and only the linear term in frequency is usually retained. A rigorous mathematical treatment of adiabatic quantum pumping¹² recovered the BPT formula given in.⁷ Within this framework the relation between resonant transmission and quantized pumped charge in an unbiased turnstile was analyzed.¹⁰ An extended scattering formalism for studying both adiabatic and non-adiabatic quantum pumping was developed in Ref. 9 and uses the Floquet theory and an S matrix depending on two-energies. Recently Mahmoodian *et al.*¹³ have computed the stationary current for a quantum wire submitted to alternating δ -like voltages. It was shown there that the current displays multiphoton peaks as a function of the Fermi momentum of the leads.

Using the Green-Keldysh formalism Q-f Sun and T. S. Lin¹⁴ have computed the current through a single level quantum dot when rectangular or harmonic potentials are applied at the contact to the leads. As it is well known, this model is exactly solvable within the wide-band limit (WBL) approximation since the Dyson equation for the retarded Green function is greatly simplified due to the leads' self-energy which within WBL is simply a delta-function.¹⁵ Later on Wang *et al.* used the Keldysh approach to investigate the non-adiabatic charge pump-

ing in the presence of photon-assisted tunneling. The explicit calculation was done within WBL and for an unbiased double barrier pump driven by a local sinusoidal signal. It was shown that at large frequencies a nonvanishing current is generated even with a single-parameter perturbation. Moreover, a sign change of the pumped current was reported when the Fermi level of the leads crosses the eigenvalues of the system. This feature was predicted also by Büttiker and Moskalets.⁹

Further progress was achieved by L. Arrachea for tight-binding models and periodic potentials.¹⁷ The method developed in this paper allows the calculation of the d.c. component of the pumped current once the partial Fourier transform (i.e. the Fourier transform with respect to one time only) of the Green functions is known. It was shown that the d.c. component can be related to a transmission function $T(\omega)$ which is interpreted as the difference between the probabilities of tunneling out from and into the system. The numerical simulations are performed for unbiased one-dimensional pumps and the pumping potential is described by a diagonal time-dependent term added to the energy at the contact sites. For two harmonic potentials the retarded Green function is computed perturbatively for weak pumping amplitude and pumping frequency. The connection between the Floquet scattering and the Green-Keldysh function formalism for time-dependent transport was discussed in Ref.18.

Besides the scattering theory and NEGF approach the pumping problem can be addressed via time integration of the Schrödinger equation by the Crank-Nicolson approximation, as proposed by Stefanucci *et al.* in a series of papers.^{19,20} Their setup starts from the ground state of the unperturbed but *coupled* system and has therefore the advantage of introducing naturally the bias as a perturbation. We remind that the Keldysh formalism requires a partitioning of the system into ‘central region’ and ‘leads’, the perturbation being the coupling between them which is established usually adiabatically in the remote past.²² The Keldysh approach is however appropriate for studying the transport in the turnstile configuration which requires to connect and disconnect periodically the pump from the leads.

Recently the equation of motion method was applied to compute various currents in 1D pumps coupled to finite wires with constant chemical potentials.²¹ Such an assumption is questionable for finite systems, especially when one is interested in the long time behavior.

In this work we are primarily interested in the transient effects on the transport properties of a many-level quantum dot turnstile which is submitted to pumping potentials at $t = 0$. We believe these effects could seriously affect the transport properties of nanostructures driven by fast oscillating signals. Also, we mention that most of the previous theoretical approaches present calculations of the *stationary* averaged current which implies either to look at the long-time limit behavior¹⁹, either to consider small pumping frequencies.¹⁷ Since in the stationary

regime the transient effects are presumably washed out, one does not need to specify how and when the pumping signal is turned on. Note also that for a proper application of the Keldysh formalism it is crucial to have a well-defined equilibrium state of the decoupled system.

While in the adiabatic regime the main advantage is to express transport quantities in terms of the frozen scattering matrix up to errors of $\mathcal{O}(\omega^2)$ or even $\mathcal{O}(\omega^3)$ (see the higher order corrections in Ref. 8), the NEGF formalism covers the entire frequency range, allowing therefore an equal footing treatment of adiabatic and nonadiabatic pumping. The Green functions needed in the current formula are computed using a recently developed method²³ which solves the integral Dyson equation *exactly* by transforming it into an algebraic equation. Through this procedure the Green functions are computed taking into account all back-and-forth scattering processes.

The content of the paper is divided as follows. Section II describes the model and gives the relevant equations, as well as the considered pumping potentials; more details about the formalism should be traced back from Ref. 23. Section III is the main part of the paper and presents the numerical results and their discussion. Conclusions are summarised in Section IV.

II. THE MODEL

Within the tight-binding model which is adopted throughout this work the Hamiltonian of the system contains three terms: the semiinfinite leads (H_L), the quantum dot turnstile (H_S) and the time-dependent pumping signals $H_T(t)$:

$$H(t) = H_S + H_L + H_T(t). \quad (1)$$

H_S has a usual tight-binding form

$$H_S = \sum_{m=1}^N (\epsilon_m + V_g) d_m^\dagger d_m + \sum_{\langle m,n \rangle} t_{mn} d_m^\dagger d_n. \quad (2)$$

Here t_{mn} are hopping terms, $\langle m,n \rangle$ denotes nearest-neighbor summation over the system sites. ϵ_m is the on-site energy and the diagonal term V_g simulates a plunger gate potential applied on the system. N is the number of sites in the dot.

Following the experimental setup from Ref. 6 we describe the oscillating tunneling barriers between the dot and the leads by time-dependent hopping terms (l, r denote the left and the right lead):

$$H_T(t) = \sum_{\alpha=l,r} V_\alpha(t) (c_{i_\alpha}^\dagger d_{m_\alpha} + h.c.). \quad (3)$$

Here c_{i_α} and $c_{i_\alpha}^\dagger$ denote the annihilation/creation operators on the i -th site of the lead α which is connected via the nearest neighbor hopping V_α to the site m_α of the dot. Similarly, d_{m_α} and $d_{m_\alpha}^\dagger$ correspond to the site m_α of the dot which is coupled to the lead α .

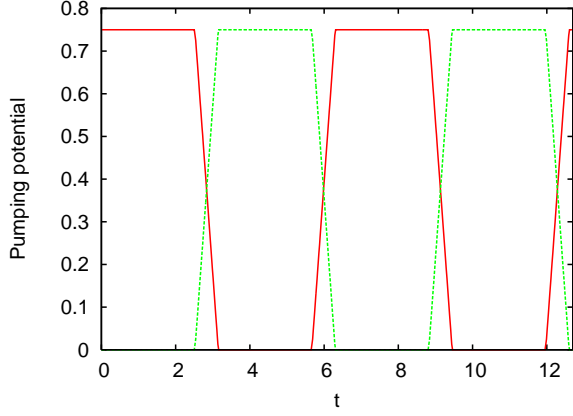


FIG. 1: (Color online) The pumping potentials applied on the left (V_l - solid line) and right (V_r - dashed line) contacts. We show two pumping cycles $k = 2$. The parameter $\Delta = 0.6$, $v_l = v_r = 0.75$ and the frequency $\omega = 1$.

The signals applied at the contacts between the dot and the leads have a trapezoidal form and are defined with the help of a function with period 2π introduced as follows (Δ is a positive number):

$$f(\omega t) = \begin{cases} 1 & \text{if } \omega t \in [0, \pi - \Delta], \\ 1 - \frac{1}{\Delta}(\omega t - (\pi - \Delta)) & \text{if } \omega t \in [\pi - \Delta, \pi], \\ 0 & \text{if } \omega t \in [\pi, 2\pi - \Delta], \\ \frac{1}{\Delta}(\omega t - (2\pi - \Delta)) & \text{if } \omega t \in [2\pi - \Delta, 2\pi]. \end{cases} \quad (4)$$

$$J_l(t) = -\frac{2e}{h} \text{Im} \left(\int_{-2t_L}^{2t_L} dE \int_0^t ds e^{-iE(s-t)} \Gamma^l(E; t, s) (G_{ll}^R(t, s) f_l(E) + G_{ll}^<(t, s)) \right). \quad (7)$$

In the above formula the retarded and lesser Green functions are given as usual in terms of Heisenberg operators $G_{ll}^R(t, t') = -i\theta(t - t') \langle \{c_{il}(t'), d_{ml}^\dagger(t)\} \rangle$ and $G_{ll}^<(t, t') = i\langle c_{il}^\dagger(t') d_{ml}(t) \rangle$. $f_l(E)$ is the Fermi function of the left lead, t_L is the hopping energy on leads and Γ^l is the linewidth depending on energy and time:

$$\Gamma^l(E; t, s) = \rho(E) V_l(t) V_l(s), \quad (8)$$

containing the pumping potentials at different times and

Then the pumping potentials of period T are given by the relations:

$$V_l(\omega t) = v_l f(\omega t) \quad (5)$$

$$V_r(\omega t) = v_r (1 - f(\omega t)), \quad (6)$$

where $\omega = 2\pi/T$ is the frequency and $v_{l,r}$ are the amplitudes of the pumping signals. It is useful to introduce the number of pumping cycles k considered in the numerical simulation. We show for clarity in Fig. 1 a train of two such pulses (i.e. $k = 2$) that we use to simulate the turnstile configuration. The quantum dot is coupled suddenly to the left lead at $t_0 = 0$ while the right contact is off. In the range $[kT/2 - \Delta, kT/2]$ the sample is simultaneously isolated from the left lead and connected to the right lead. This switching is done linearly at a slope $1/\Delta$ (note that a larger Δ implies a slower onset of the couplings). In the second halfperiod of each pumping cycle the right contact is open, allowing thus the charge pumping. The cycle is completed by lowering the left tunneling barrier (i.e. increasing $V_l(t)$) and turning off the coupling to the right lead.

As it is widely known, the standard application of the Keldysh formalism leads to the following formula for the current entering the system from the left lead (here we take for simplicity one dimensional leads; a many-channel formula and more details are to be found in Ref. 23):

the density of states at the endpoint of the semiinfinite one-dimensional lead $\rho(E)$:

$$\rho(E) = \theta(2t_L - |E|) \frac{\sqrt{4t_L^2 - E^2}}{2t_L^2}. \quad (9)$$

The retarded and the lesser Green functions are computed from the Dyson and Keldysh equations:

$$G^R(t, t') = G_0^R(t, t') + \int_0^t dt_1 G^R(t, t_1) \int_0^{t_1} dt_2 \Sigma^R(t_1, t_2) G_0^R(t_2, t') \quad (10)$$

$$G^<(t, t') = \int_0^t dt_1 G^R(t, t_1) \int_0^{t'} dt_2 \Sigma^<(t_1, t_2) G^A(t_2, t'), \quad (11)$$

where $G_0^{R,A}(t, t')$ are the retarded and advanced Green

functions of the isolated dot and $\Sigma^{R,<}$ are the retarded

and lesser self-energies. It is worth mentioning that both self-energies contain the known Green functions of the semiinfinite leads but they are also quadratic functions of the pumping potentials whose time variable is different (see Eq. 8). Therefore, their time-dependence is much more complicated than in other approaches where the pumping signals are applied to the system or to the leads and are described by diagonal terms in the Hamiltonian. In particular, the algorithm taken in Ref. 20 would be difficult to use. The time-dependent occupation number can be computed from the lesser Green function of the dot:

$$N(t) = \text{Im} \sum_{m=1}^N G_{mm}^<(t, t) = \sum_{m=1}^N N_m(t). \quad (12)$$

$N_m(t)$ are on-site occupation numbers and will be used in the next section to gain information about the internal charge dynamics during the pumping cycle. A similar formula can be written down for the current $J_r(t)$ flowing from the system towards the right lead.

As we have said, taking explicitly into account the initial instant when the pumping signals are applied leads to transient effects.²³ One consequence is that the period-averaged currents depend on the period index k . We introduce therefore a k -indexed period-average for the currents (the k -th period covers the interval $[t_{k-1}, t_k]$ and $t_0 = 0$):

$$\bar{J}_{\alpha,k} = \frac{1}{T} \int_{t_{k-1}}^{t_k} dt J_{\alpha}(t), \quad \alpha = l, r. \quad (13)$$

Although the approach taken in this work does not include the electron-electron interaction it captures the basic known features of turnstile pumps: the quantized pumped charge in low frequency regime and the satellite peaks due to photon-assisted tunneling in high-frequency regime. Moreover, most of the results are presented at rather strong coupling to the leads when the dot is fairly open and the Coulomb blockade effects are not important. In a recent work Splettstoesser *et al.*²⁴ proposed a method for dealing with Coulomb interactions in adiabatic quantum pumps. This approach is based on the quantum Master equation and uses a perturbative expansion in the tunnel coupling. In the case of the unbiased quantum dot turnstile these authors found that one has to consider the second order term in the tunnel coupling to get a non vanishing pumping.

III. NUMERICAL SIMULATIONS

In this section we present the main numerical results and discuss the transport properties of the turnstile pump in different regimes. The bias, the frequency, the energy, the hopping constants on the leads, the coupling strengths and the gate potential will be expressed in terms of the hopping energy of the central region t_D which is chosen as energy unit.

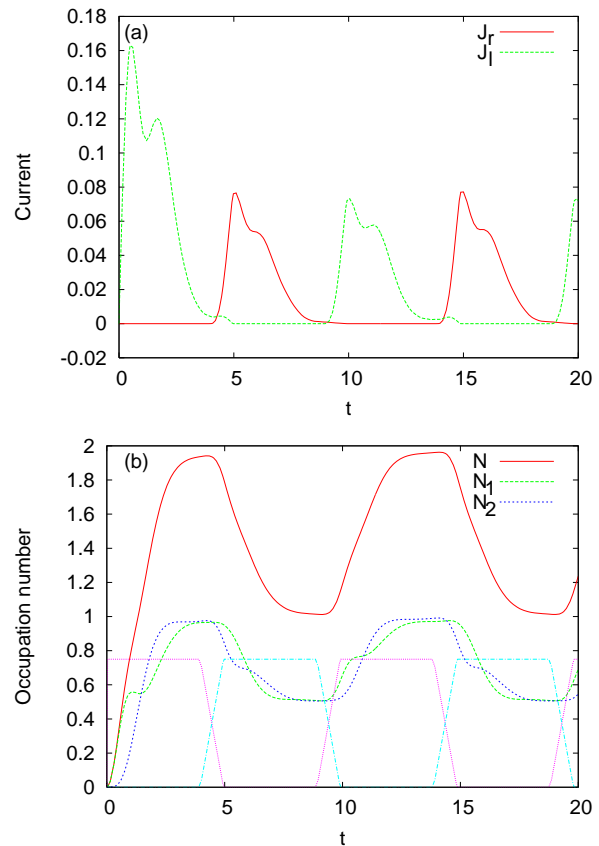


FIG. 2: (Color online) (a) The pumped current in the right lead (J_r) and the current entering the system from the left lead (J_l) for a 2-site turnstile. (b) The occupation number of the dot $N(t)$ and the on-site occupations $N_i(t)$, $i = 1, 2$. The pumping potentials are also given. During the second halfperiod of each pumping cycle the turnstile expells one electron to the right lead. The bias is fixed to $W = 3.0$, $\omega = 0.6$, $v_l = v_r = 0.75$ and $kT = 0.0001$.

The current is therefore given in units of et_D/\hbar and the time expressed in units of \hbar/t_D . We take $e = \hbar = 1$. The bias window (BW) is defined as the difference between the chemical potentials of the leads $W = \mu_l - \mu_r$. To make a connection to physical units one could take for example the energy unit as $t_D = 0.1$ meV. Then the frequency unit would be $\omega \sim 25$ GHz and the time unit $t \sim 7$ ps. The thermal energy $kT = 0.0001$ in all numerical simulations.

We consider first a two-site one-dimensional turnstile submitted to a finite bias and modulated by the trapezoidal signal introduced in Section II. In order to simulate the conditions of the experiment performed by Kouwenhoven *et al.*⁶ we set the bias window to $W = 3.0$ with respect to the chemical potential of the right lead $\mu_r = 0$ such that the highest level of the isolated dot $E_1 = 1$ is located in it. Fig. 2a shows the current $J_l(t)$ from the left lead towards the turnstile and the current $J_r(t)$ pumped into the right lead during two pumping cycles. The frequency is $\omega = 0.6$ and the maximum height of the tun-

neling barriers is $v_l = v_r = 0.75$. As expected, a nonvanishing current is generated in the right lead during the second halfperiod of each pumping cycle. The pumping mechanism is proved by the behavior of the occupation number $N(t)$ which is given in Fig. 2b. At the beginning of the first cycle the system collects charge from the left lead and since the coupling to the right lead is zero there are almost two electrons in the system after one halfperiod. We shall call this halfperiod the charging halfperiod. The charge dynamics within the system is also given in Fig. 2b through the occupation numbers of the two sites N_1 and N_2 . For the clarity of discussion we have also included in the figure the two potentials applied on the leads. The first site is rapidly populated up to 0.5 and then stays at this occupation while the second site starts to be filled. The current J_l decreases in this short time range.

Then we see that N_2 increases faster than N_1 and both are reaching a constant value. Due to the small frequency considered here the halfperiod of the pumping cycle exceeds the time needed for the system to be completely filled with electrons and therefore, as long as the coupling to the right lead is still turned off, the total occupation number is steplike. The current J_l becomes very small in this range because as both sites are filled it is more difficult to inject charge (notice the lower slope at which N_1 increases). The pumping starts effectively in the second half of the cycle and leads to the transmission of one electron in the right lead, as observed in Ref. 6. During the pumping halfperiod the occupation of the right contact drops quickly to 0.75 but then decreases at a lower rate as the first site is depopulating. Note that in the pumping sequence N_1 drops more rapidly than N_2 . The occupation number at the end of the pumping cycle does not decrease below 1 because the lowest level of the dot $E_2 = -1$ is well below the bias window and cannot contribute to transport.

From the above discussion it is clear that the efficiency of the pump depends on two facts: first, the charging halfperiod should allow the complete filling of the turnstile and second, the levels within the bias window must be entirely depopulated during the pumping halfperiod. In the intermediate regime $\omega \sim V_{l,r}$ (not shown) the system still transfers one electron, the difference being that the occupation number decreases faster and more abruptly than in Fig. 2. The transient effects on the time-dependent currents and pumped charge that appear as the pumping frequency increases are captured in Figs. 3a-d. At $\omega = 1.25$ the shape of the currents is similar to the one in Fig. 2a. However, the current pumped during the first cycle is smaller than the ones corresponding to the next cycles and the occupation number plotted in Fig. 3d shows that less charge is pumped. Also, there are no more steps in $N(t)$. The behavior of the occupation number helps us to identify the new features of the charge dynamics in the nonadiabatic regime.

On the other hand, the coupling to the right lead closes before the level within the bias window depopulates. As

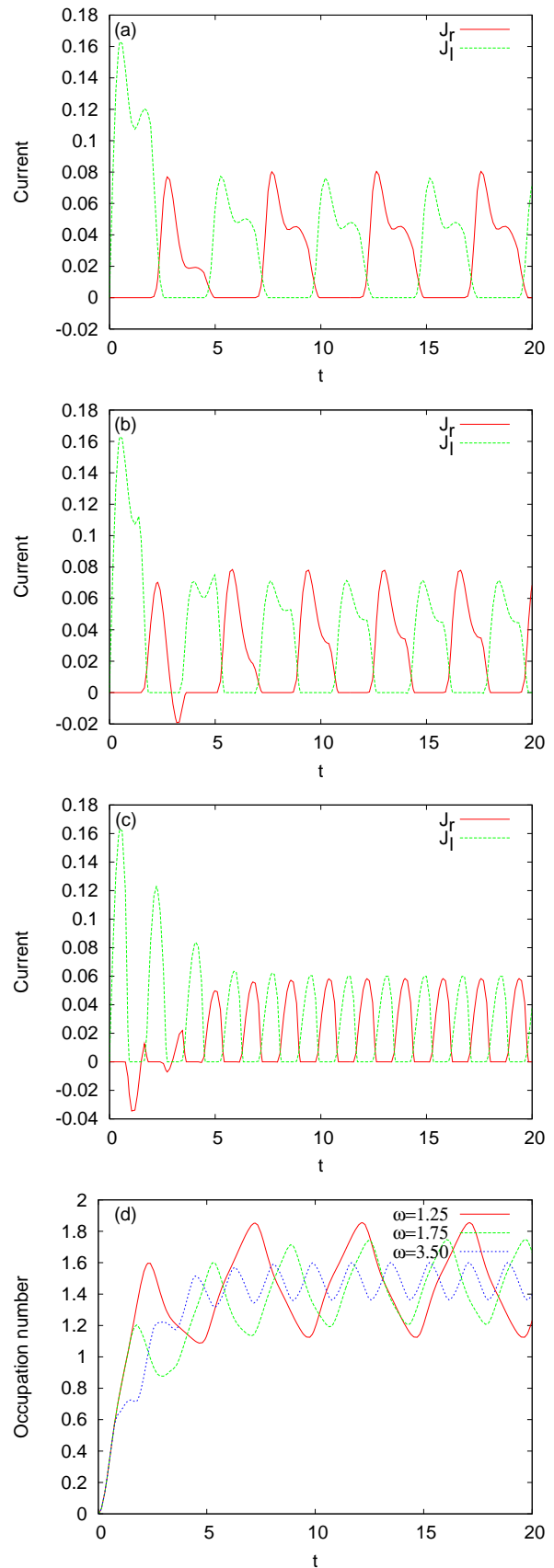


FIG. 3: (Color online) The shape of the currents J_r and J_l depends on the pumping frequency: (a) $\omega = 1.25$, (b) $\omega = 1.75$, (c) $\omega = 3.5$. At large frequency J_r takes negative values in the first pumping cycles. (d) The occupation number $N(t)$ corresponding to the three frequencies taken in (a), (b), (c). $W = 3.0$, $v_l = v_r = 0.75$, $kT = 0.0001$.

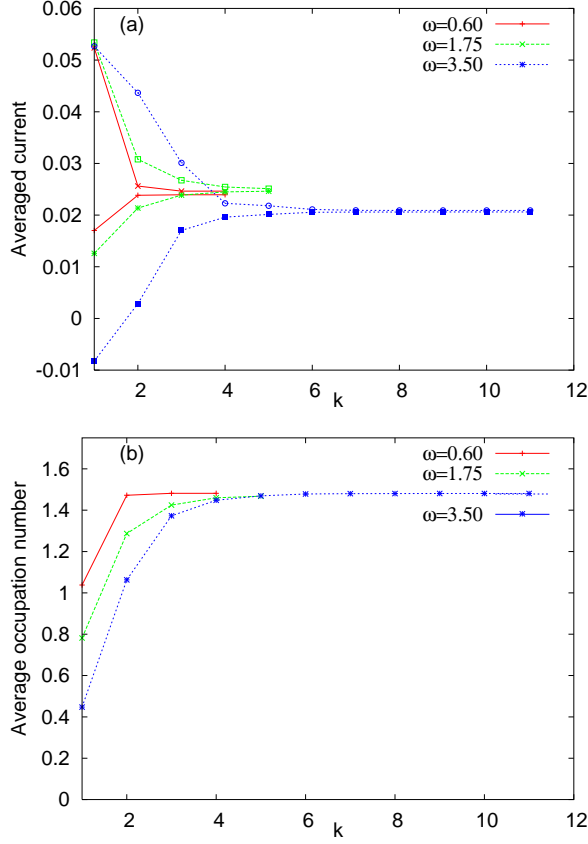


FIG. 4: (Color online) (a) The average currents $\bar{J}_{r,k}$ and $\bar{J}_{l,k}$ as a function of the period index k . There are three pairs of curves, corresponding to the frequencies $\omega = 0.6$ ($k = 4$), $\omega = 1.75$ ($k = 5$) and $\omega = 3.5$ ($k = 11$). For each frequency the two averaged currents are drawn with the same type of line (color); \bar{J}_r (\bar{J}_l) has a positive (negative) slope. (b) The average occupation number (see the discussion in the text). $W = 3.0$, $v_l = v_r = 0.75$, $kT = 0.0001$.

a consequence, at the end of the pumping cycle there is a residual charge (~ 0.1) which is stuck within the bias window. By further increasing the frequency up to $\omega = 1.75$ another effect appears in Fig. 3b. Although there is a nonvanishing pumped current during the first cycle J_r takes negative values at the end of the cycle, which means that in this interval the system absorbs charge rather than pumps it. Looking at the corresponding occupation number in Fig. 3d one infers why the system does not act like a pump over the entire pumping sequence. $N(t)$ goes slightly above 1 then drops to 0.9; during this interval the system pushes electrons to the right lead and therefore $J_r(t) > 0$. Then the occupation number increases, leading to negative values of $J_r(t)$ (the pumping period in Fig. 3b is 3.7). The physical picture behind this is the following: i) In the first halfperiod both levels are populated, though not completely; ii) During the first part of the pumping sequence the level within the bias window depopulates, generating therefore a positive current J_r ; iii) When this happens the total occupation number

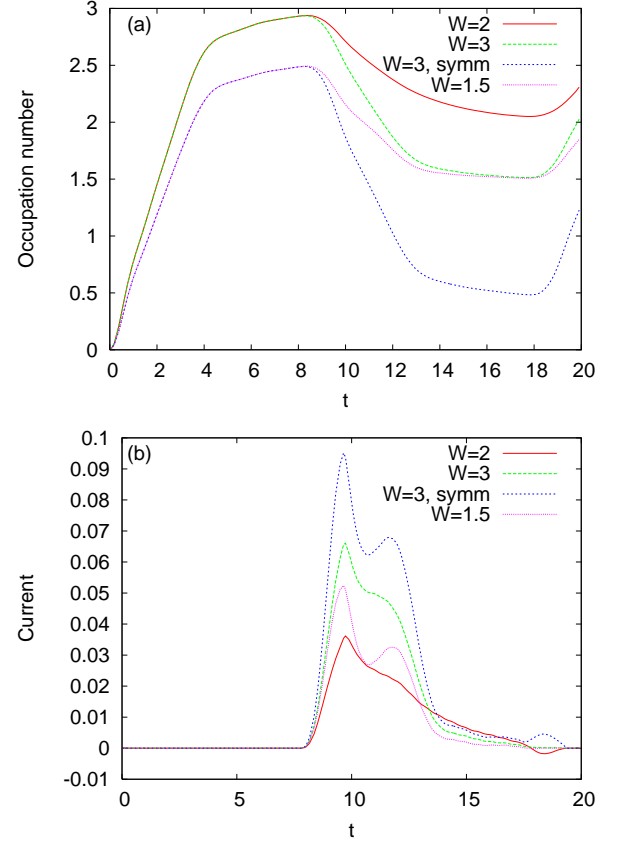


FIG. 5: (Color online) (a) The occupation number at different values of the bias window and different alignment of the turnstile levels with respect to the bias window. (b). The pumped current $J_r(t)$ corresponding to the occupation numbers in (a). For all curves the frequency is set to $\omega = 0.3$. We show only the first pumping cycle.

goes below 1; also, since the chemical potential of the right lead is higher than the lower level of the dot, the system absorbs charge from the right lead and the occupation number increases again.

Finally, Fig. 3c shows the currents in a highly non-adiabatic regime $\omega = 3.5$. The steplike features within each pumping cycle are washed out and on the first cycle the system does not pump any charge (the occupation number is simply increasing and stays below 1). Moreover, even when a stable pumping regime is achieved (for $t > 5$) it is not effective at all since very little charge is pumped.

The transient regime should be noticed as well in the period-averaged currents. In order to check this we give in Fig. 4a these currents for the three frequencies considered in Fig. 3. The following things are observed: i) In all three cases the d.c. components of the currents become eventually equal and their value does not depend anymore on the period index. Moreover, the averaged current is conserved. The passage to this ‘stationary’ regime is faster at low frequencies; ii) In the transient regime $\bar{J}_{l,k}$ exceeds $\bar{J}_{r,k}$ since there is a net charge ac-

cumulation in the dot along each transient cycle (see the occupation numbers in Fig. 3d); iii) At large frequencies $\bar{J}_{r,k}$ takes negative values in the transient regime (see the first cycle at $\omega = 3.5$) because the system absorbs charge from the right lead.

Fig. 4b shows that the average occupation number depends strongly on the period index in the transient regime and settles down to 1.5 in the long-time limit. Notice that this means that the level which contributes to the transport is half occupied.

The bias applied on the leads is an important parameter in turnstile operation because it controls the number of levels giving the main contribution to the current. As reported experimentally⁶ the number of electrons pumped during one pumping cycle is given by these levels. Fig. 5a shows the occupation numbers of a three sites turnstile pump submitted to a different bias. We take a small frequency ($\omega = 0.3$) and therefore the pumping cycle is long enough to allow the filling of the lowest levels (the dot has three eigenstates $E_{\pm} = \pm 1.4$ and $E_0 = 0$). For $\mu_l = 3$ and $\mu_r = 1$ only the highest level is located within the bias window and the pump transfers one electron. The occupation number at the end of the cycle is $N = 2$. We emphasize that the frequency is much smaller than the gap between E_0 and E_- and therefore the lowest level cannot give an important contribution to the current via excited sidebands.

By decreasing the chemical potential of the right lead to $\mu_r = 0$ the middle level aligns to μ_r and the turnstile pumps 1.5 electrons at $W = 3$. Note that due to the rather large coupling to the leads there is no charge quantization condition to be fulfilled. The dotted line shows the occupation number for the same bias W with $\mu_l = 1.5$ and $\mu_r = -1.5$. In this case we have a symmetric bias window (as marked in the figure) containing the middle level in the center. The other two levels are close to the chemical potentials of the leads. The transferred charge is $Q_p \sim 2$, suggesting that each level aligned to one chemical potential pumps only half electronic charge. This happens because the level close to μ_r (μ_l) are difficult to depopulate (populate). Also, by tuning the width and the position of the bias window it is possible to transfer the same charge in different ways (i.e. by involving different levels of the pump). For example, setting $\mu_l = 1.5$ and $\mu_r = 0$ one can still transfer one electron at a bias window $W = 1.5$. Of course, the efficiency of the pump increases when the number of levels participating in transport increases. Fig. 5b shows the pumped currents associated to the occupation numbers in Fig. 5a. Although both cases $W = 1.5$ and $W = 2$ correspond to a pumped charge $Q_p = 1$, the current is higher at $W = 1.5$. Note also that the currents have a peak structure when two levels participate in transport.

The discussion around Figs. 3 and 4 suggests that at a given frequency the transient regime would cover more pumping cycles if the number of levels located below the bias window increases. This is confirmed in Fig. 6 which shows the occupation number of a 3-site turnstile. We

take $\mu_l = 3$ and $\mu_r = 1$ and in this case the BW contains only the highest level $E_+ = 1.4$.

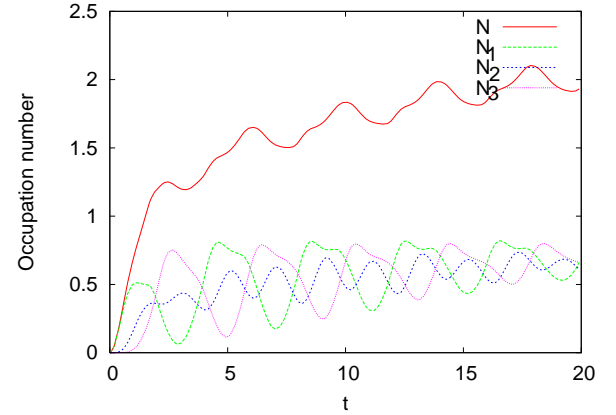


FIG. 6: (Color online) (a) The total occupation number $N(t)$ and the on-site occupation numbers N_i ($i, 1, 2, 3$) for a 3-site turnstile submitted to a bias $W = 2$ and to a pumping signal of frequency $\omega = 1.57$.

$N(t)$ shows clearly that the other two levels are filled only after $k = 5$ pumping cycles. Notably, even in the transient regime the system pumps a small amount of charge (~ 0.25) because of the highest level from the BW. This level cannot be completely filled in the transient cycles because most of the charge populates the lowest two levels. The behavior of the individual occupation numbers N_i , $i = 1, 2, 3$ confirms the intuitive picture of the internal charge dynamics. It is easily seen that for any pumping cycle except the first, the occupation number of the 3rd site decreases even in the first halfperiod, namely during the charging process. Since in this time range the contact to the right lead is turned off the charge from the right contact can only flow back to the middle site. Indeed, N_2 increases as N_3 decreases.

As the dot charges from the left lead the inverse flow is noticed. In the pumping halfperiod the middle site occupation firstly increases because the charge accumulated in the first site passes to the right contact which is now open, and finally decreases. All these internal bouncing trajectories are taken accurately into account in our calculation because the method we used to solve for the Dyson equation gives the *entire* matrix of the Green function (not only the diagonal matrix elements entering the current formula).

We turn now to another important feature of time-dependent transport, namely the contribution due to inelastic scattering processes in which the incident electrons gain or loose energy quanta from the driving fields. Within the Floquet scattering approach it was shown^{9,25} that the outgoing electrons can have any energy $E_n = E + n\hbar\omega$ in the so called sideband ladder, E being the energy of the incident electrons. In the present model the pumping potential is *not* periodic because of the condition $V_l(t) = V_r(t) = 0$ for $t < 0$, therefore the Floquet theorem cannot be rigorously applied. At best, one

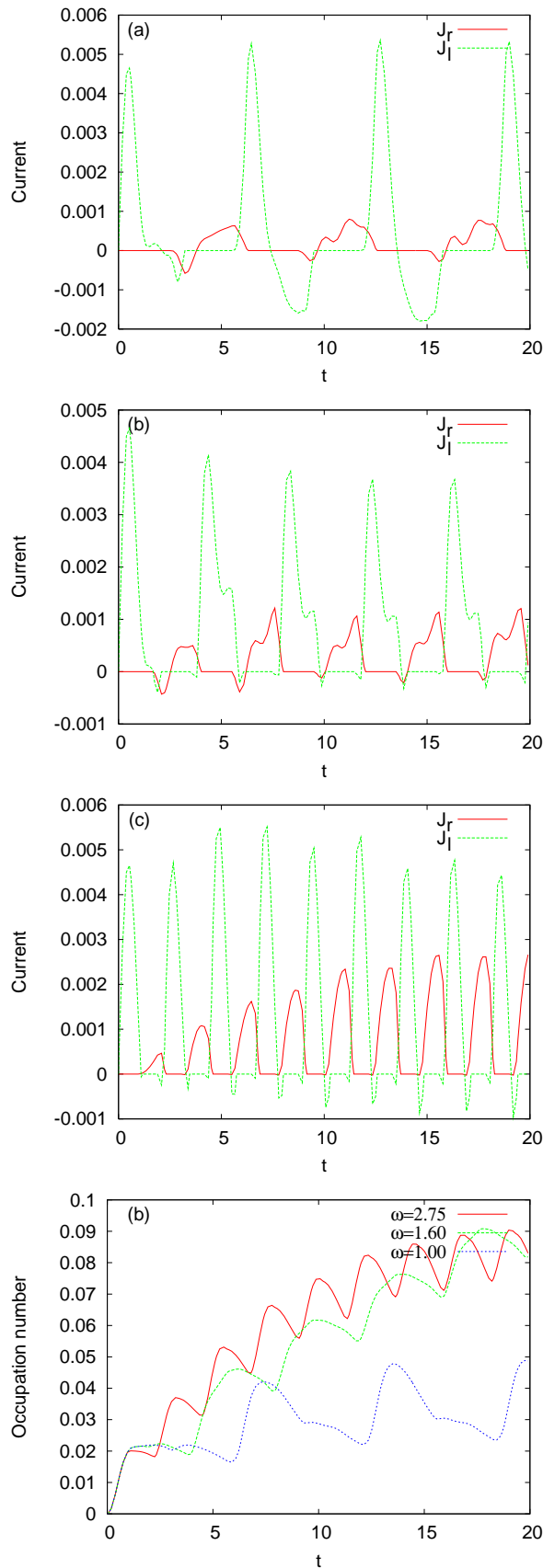


FIG. 7: (Color online) For a 3 site turnstile with all the levels above the bias window one can notice sideband contributions to the two time-dependent currents at frequency (a) $\omega = 1.0$, (b) $\omega = 1.6$ and (c) $\omega = 2.75$. (d) The occupation number at different values of the frequency.

can use results of the Floquet theory in the long time limit where all relevant quantities will oscillate with the frequency of the driving signals (see Ref. 26 for a discussion). Nevertheless, inelastic tunneling processes are physically possible especially in the transient regime and should be noticed in the averaged currents. In particular one expects to see additional contributions to the current at frequencies matching the gaps $\mu_{l,r} \pm E_i$ between the levels of the isolated system and the chemical potentials of the leads.

In order to check these features we tune the bias window *below* the three levels of the 3-site pump by setting $\mu_l = -2.5$ and $\mu_r = -3.5$ such that $E_- - \mu_l \sim 1$. We take a small pumping amplitude $v_l = v_r = 0.35$ and look at the currents for several frequencies, as shown in Figs. 7a-d. For small frequencies ($\omega = 0.3$ and $\omega = 0.5$ - not shown) there is no pumped current and J_l takes both positive and negative values, while $N(t)$ increases and decreases accordingly during the charging halperiod. This suggests that the system repels incident electrons back to the left lead. This happens because on one hand there is no level below or within the bias window and, on the other hand, the frequency is too small to allow the population of the lowest level. The situation changes for $\omega = 1$ (see Fig. 7a). A pumped current appears in all three cycles presented. We related this to the occupation number plotted in Fig. 7d which shows that there is a charge pumped into the right lead. When comparing Fig. 7a and Fig. 7d (the dotted line) one notes that in the second half of the charging cycle $J_l < 0$ and $N(t)$ decreases. This signals the energy relaxation process from the lowest level of the system to the left lead only, because the contact to the right lead is not yet open. Only the second (lower slope) decrease of $N(t)$ is associated to pumping through the right lead. At $\omega = 1.6$ (Fig. 7b) the pumped charge and current increase. J_l is mostly positive because the fast oscillating signals prevent relaxation to the left lead. The pumped current still shows a peak structure. In Fig. 7c we show a highly non-adiabatic regime at $\omega = 2.75$. In this case the second level $E_0 = 0$ will contribute as well. In order to avoid tunneling from the right lead to the level E_- we have considered for this curve $\mu_r = -5$. The peak structure of the pumped current disappears and a periodic regime establishes slowly after 9 cycles. As we have said in the introduction, the present approach takes into account all tunneling processes between the leads and the system and within the system. This nonperturbative treatment might be crucial for describing the relaxation processes mentioned above, especially in the transient regime where the resonances are not well defined.

Finally we investigate briefly the satellite peaks appearing in the averaged current when a gate potential is used to move the levels of the dot. These peaks were observed experimentally³ and are associated with absorption and emission processes of energy quanta from the pumping fields. Theoretically they were obtained first in the Master equation framework.²⁷ In the Keldysh formal-

ism a calculation of the stationary current in the WBL approximation was also present in Ref. 28. Here we want to check whether the satellite peaks appear also in the first pumping cycles, namely in the transient regime. To this end we consider the dependence of the pumped current for a two site turnstile on a gate potential V_g (see the Hamiltonian given in the introduction) which shifts the two levels of the isolated system. Since we are interested in observing satellite peaks associated to one level only we take the parameters such that $v_{l,r} < \omega < \delta 2$, where $\delta = E_1 - E_2 = 1$ is the level spacing. Fig. 8a shows the averaged current associated to the 2nd pumping cycle. One notices as once two satellite peaks located on each side of main resonant peaks (at $V_g = \pm 1$ the levels of the isolated dot are shifted to zero, therefore they are located in the middle of the bias window). Also, the distance between the satellite peaks and the associated main peak equals roughly the frequency $\omega = 0.65$ and confirms the absorption/emission picture. There are however several aspects due to the transient regime in which these peaks appear. i) As shown in Fig. 8b the averaged current on the first pumping cycle does not display satellite peaks and is mostly negative. ii) Also, in Fig. 8a the first satellite peak has a negative value. This can be understood by looking at Fig. 8c which gives the 3D plot of the pumped current as a function of time and gate potential. Clearly, around $V_g = -1.65$ there is a maximum positive current at the beginning of the pumping cycle. In this range the system effectively pumps charge to the right lead via photon assisted tunneling involving the highest level of the dot. This process is rather weak because in the transient regime the occupation of the levels below the bias window is not complete. This is why after a short pumping regime the system absorbs charge from the lead and therefore $J_r(t) < 0$. As the first level enters the bias window a main peak appears around $V_g = 0$. Similar description can be made for the contribution of the second level. iii) For $V_g > 0.3$ the average current is positive; the photon-assisted tunneling contribution to the pumping process is amplified and the current vanishes as the lowest level of the dot is pushed upwards.

Our calculations show that photon assisted tunneling takes place also in the transient regime.

IV. CONCLUSIONS

We have studied the turnstile pump regime of a few level noninteracting quantum dot within the non-equilibrium Green-Keldysh formalism for time-dependent transport. The out-of-phase oscillating barriers coupling the system to the leads are described by time-dependent hopping terms. In the numerical calculations we have considered a train of trapezoidal pulses that mimic the configuration used in the experimental work of Kouwenhoven *et al.*⁶. Our approach includes explicitly the starting time of the pumping cycles and therefore captures the transient behavior of the time-

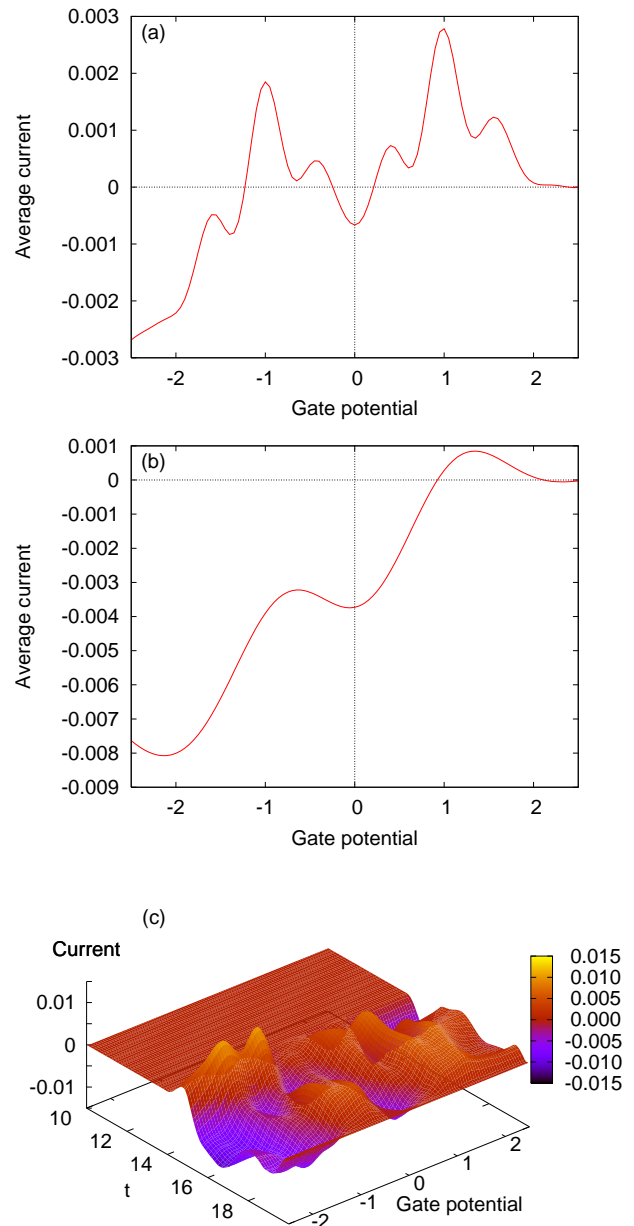


FIG. 8: (Color online) (a) The averaged current $\bar{J}_{r,2}$ as a function of the gate potential for a two sites turnstile shows satellite peaks associated to photon-assisted tunneling during the second pumping cycle. (b) The averaged current corresponding to the first pumping cycle $\bar{J}_{r,1}$ does not contain satellite peaks. (c) The current J_r as a function of time (only the second cycle is shown) and gate potential. The discussion is made in the text. Other parameters $\omega = 0.65$, $v_l = v_r = 0.35$, $\mu_l = 0.2$, $\mu_r = -0.2$, $kT = 0.0001$.

dependent and period-averaged current. To our best knowledge, such a calculation is presented here for the first time. We identify basically two stages of transport. The system experiences first a transient regime with poor pumping efficiency. This is due to the fact that the dot

rather absorbs charge from the leads in order to populate the levels located below the bias window. The number of pumping cycles in which the transient features should be observed in future experiments with many level turnstiles increases if the bias window contains only the highest levels. In the second stage the occupation number of the dot and the currents oscillate with the pumping period. We show that at low frequency and strong coupling to the leads an integer or half-integer number of electrons are pumped, depending on the number and the location of the levels within the bias window. In the high-frequency case the pumped charge is rather small even if additional contributions appear due to scattering processes involving energy sidebands. We show that satellite peaks due to the photon-assisted tunneling appear also

in the transient regime. The present analysis could be extended to two-dimensional systems in order to discuss magnetic field effects. Also, different types of potentials (e.g. harmonic or damped pulses) can be considered.

Acknowledgments

This work was supported in part by the Icelandic Science and Technology Research Programme for Postgenomic Biomedicine, Nanoscience and Nanotechnology. V.M was also supported by CEEEX Grant D11-45/2005. We acknowledge useful discussions with C. S. Tang.

-
- ¹ M. Switkes, C. M. Marcus, K. Campman, and A. C. Gosard, *Science* **283**, 1905 (1999).
 - ² L. J. Geerligs, V. F. Anderegg, P. A. M. Holweg, J. E. Mooij, H. Pothier, D. Esteve, C. Urbina and M. H. Devoret, *Phys. Rev. Lett.* **64**, 2691 (1990).
 - ³ W.G. van der Wiel, T.H. Oosterkamp, S. de Franceschi, C.J.P.M. Harmans, and L.P. Kouwenhoven. *Strongly Correlated Fermions and Bosons in Low-Dimensional Disordered Systems*, eds. I.V. Lerner et al., pp.43-68 (2002), Kluwer Academic Publishers.
 - ⁴ H. J. Krenner, S. Stuffer, M. Sabathil, E. C. Clark, P. Ester, M. Bichler, G. Abstreiter, J. Finley and A. Zrenner, *New J. Phys.* **7**, 184 (2005).
 - ⁵ T. Fujisawa, D. G. Austing, Y. Tokura, Y. Hirayama, S. Tarucha, *J. Phys. Cond. Mat.* **15**, R1395 (2003).
 - ⁶ L. P. Kouwenhoven, A. T. Johnson, N. C. van der Vaart, C. J. P. M. Harmans, and C. T. Foxon, *Phys. Rev. Lett.* **67**, 1626 (1991).
 - ⁷ P. W. Brouwer, *Phys. Rev. B* **58**, R10135 (1998).
 - ⁸ O. Entin-Wohlman, A. Aharony, and Y. Levinson, *Phys. Rev. B* **65**, 195411 (2002).
 - ⁹ M. Moskalets and M. Büttiker, *Phys. Rev. B* **66**, 205320 (2002).
 - ¹⁰ O. Entin-Wohlman and A. Aharony, *Phys. Rev. B* **66**, 035329 (2002).
 - ¹¹ S. Kohler, J. Lehmann, P. Hnggi, *Phys. Rep.* **406**, 379 (2005).
 - ¹² J.E. Avron, A. Elgart, G.M. Graf, and L. Sadun, *Comm. Pure and Appl. Mathematics* LVII, 0538 (2004), *Phys. Rev. Lett.* **87**, 236601 (2001).
 - ¹³ M. M. Mahmoodian, L. S. Braginsky, and M. V. Entin, *Phys. Rev. B* **74**, 125317 (2006), *JETP* **100**, 920 (2005).
 - ¹⁴ Q-f Sun, T-h Lin, *J. Phys. Cond. Mat* **9** 3043 (1997).
 - ¹⁵ A.-P. Jauho, N. S. Wingreen, and Y. Meir, *Phys. Rev. B* **50**, 5528 (1994).
 - ¹⁶ B. Wang, J. Wang, and H. Guo, *Phys. Rev. B* **68**, 155326 (2003).
 - ¹⁷ L. Arrachea, *Phys. Rev. B* **72**, 125349 (2005).
 - ¹⁸ L. Arrachea, M. Moskalets, *Phys. Rev. B* **74**, 245322 (2006).
 - ¹⁹ S. Kurth, G. Stefanucci, C.-O. Almbladh, A. Rubio, and E. K. U. Gross, *Phys. Rev. B* **72**, 035308 (2005), G. Stefanucci, C.-O. Almbladh *Phys. Rev. B* **69**, 195318 (2004).
 - ²⁰ G. Stefanucci, S. Kurth, A. Rubio, E. K. U. Gross, *cond-mat/0701279*.
 - ²¹ A. Agarwal, D. Sen, *J. Phys. Condens. Matter* **19** 046205, (2007).
 - ²² C. Caroli, R. Combescot, P. Nozieres, and D. Saint-James, *J. Phys. C* **4**, 916 (1971).
 - ²³ V. Moldoveanu, V. Gudmundsson, A. Manolescu, *cond-mat/0703179*.
 - ²⁴ J. Splettstoesser, M. Governale, J. König, and R. Fazio, *Phys. Rev. B* **74**, 085305 (2006).
 - ²⁵ M. Wagner, *Phys. Rev. A* **51**, 798 (1995), *Phys. Rev. B* **49**, 16544 (1994).
 - ²⁶ D. W. Hone, R. Ketzmerick, and W. Kohn, *Phys. Rev. B* **56**, 4045 (1997).
 - ²⁷ C. Bruder and H. Schoeller, *Phys. Rev. Lett.* **72**, 1076 (1994).
 - ²⁸ Q-f Sun, J. Wang, and T-han Lin, *Phys. Rev. B* **58**, 13007 (1998).